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Excitons and exciton oscillator strengths in two-dimensional superlattices

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Abstract. We have calculated excitonic Bloch states in a quantum well with a two-dimensional (2D) periodic potential. For the potential parameters used the two lowest states can be well described in the tight-binding approach while the higher states represent free excitons affected by the periodic potential. The redistribution of oscillator strengths for bound-like and free-like excitons with varying the period has been also analyzed.

The resonant optical reflection from a lateral array of quantum dots was calculated in [1] for particular limiting cases, namely, for short-period structures or in the constant-field approximation. Analytical results for arbitrary relation between the lateral period a and the light wavelength as well as between the exciton radiative and nonradiative damping rates have been presented recently in [2]. The theories [1, 2] are derived neglecting the overlap of the exciton envelope functions excited at different dots. In the present work we extend the theory allowing an exciton to tunnel coherently from one potential minimum to another.

We consider a quantum well (QW) with a periodic two-dimensional (2D) potential $V(x, y) = V(x + a, y) = V(x, y + a)$ acting at an exciton as at a single particle and making no effect on the exciton internal state, i.e. x, y are the in-plane coordinates of the exciton center-of-mass. For simplicity, we assume the potential $V(x, y)$ to have the point symmetry of a quadrate: $V(x, y) = V(\pm x, \pm y) = V(y, x)$. Due to the potential $V(x, y)$ the exciton energy spectrum is transformed from the parabolic dispersion $E_{exc}(k_x, k_y) = \hbar^2(k_x^2 + k_y^2)/(2M)$ in an ideal QW with $V \equiv 0$ into a series of 2D minibranches (M is the exciton in-plane translational effective mass).

Under normal incidence of the light only the Γ_1 excitonic states with $k_x = k_y = 0$ are excited. We enumerate these states by the index ν. The corresponding envelope functions, $\psi^\nu(x, y)$, of the exciton translational motion are periodic and invariant under all quadratic symmetry operations. They can be expanded in the Fourier series

$$\psi^\nu(x, y) = \frac{1}{a} \sum_{lm} c_{lm} \exp\left[i\frac{2\pi}{a}(lx + my) \right], \tag{1}$$

where l, m are integers $0, \pm 1 \ldots$ We choose the normalization condition $\int_{\Omega_0} |\psi|^2\, dxdy = 1$, where Ω_0 is the unit cell, say the area $-a/2 < x, y < a/2$. Thus, the expansion coefficients c_{lm} satisfy the condition $\sum_{lm} |c_{lm}|^2 = 1$, whence

$$\sum_{lm} c_{lm}^{(\nu)*} c_{lm}^{(\nu')} = \delta_{\nu\nu'} \,. \tag{2}$$

Let us consider a pair of integers l, m as a two-component vector and denote the star of the vector (l, m) as β. The star contains the vectors $(\pm l, \pm m)$ and $(\pm m, \pm l)$. For $l \neq m \neq 0$ the star consists of eight vectors, otherwise it has four different vectors (if

$l = m \neq 0$ or $l = 0, m \neq 0$ or $l \neq 0, m = 0$) and one vector in the particular case $l = m = 0$. Note that, for the Γ_1 states, the coefficients c_{lm} in Eq. (1) with l, m belonging to the same star coincide: $c_{l,m} \equiv c_\beta$. In the method of plane waves defined by Eq. (1) the Schrödinger equation reads

$$\left[\frac{\hbar^2}{2M}\left(\frac{2\pi}{a}\right)^2 \beta^2 - E\right] c_\beta + \sum_{\beta'} c_{\beta'} \sum_{(l',m')\in\beta'} V_{lm,l'm'} = 0\,, \tag{3}$$

$$V_{lm,l'm'} = \frac{1}{a^2}\int_{\Omega_0} V(x,y)\,\cos\left\{\frac{2\pi}{a}[(l'-l)x + (m'-m)y]\right\} dxdy\,,$$

where $\beta^2 = l^2 + m^2$, E is the energy referred to the bottom of the exciton band in an ideal QW. Now we define the lateral potential as a periodic array of disks, namely,

$$V(x,y) = \sum_{lm} v(x - la, y - ma)\,, \tag{4}$$

$$v(x,y) \equiv v(\rho) = \begin{cases} -v_0\,, & \text{if } \rho \le R \\ 0\,, & \text{if } \rho > R\,, \end{cases}$$

where $\rho = \sqrt{x^2 + y^2}$. Then one has

$$V_{lm,l'm'} = -v_0 \frac{R}{a}\,\frac{J_1\left(2\pi\sqrt{(l'-l)^2 + (m'-m)^2}\,R/a\right)}{\sqrt{(l'-l)^2 + (m'-m)^2}}\,, \tag{5}$$

where $J_1(t)$ is the Bessel function.

For the sake of convenience we introduce the dimensionless variables

$$\varepsilon = \frac{E}{E_0}\,,\; u_0 = \frac{v_0}{E_0}\,,\; \mu = \frac{R}{a}\,, \quad \text{where} \quad E_0 = \frac{\hbar^2}{2M}\left(\frac{2\pi}{R}\right)^2\,, \tag{6}$$

and the coefficients

$$C_\beta = \sqrt{n_\beta}\, c_\beta\,, \tag{7}$$

where n_β is the number of vectors in the star β. Then we can rewrite Eq. (3) in the dimensionless form as

$$(\mu^2\beta^2 - \varepsilon)C_\beta - u_0 \sum_{\beta'} U_{\beta\beta'} C_{\beta'} = 0\,, \tag{8}$$

$$U_{\beta\beta'} = -\frac{1}{v_0\sqrt{n_\beta n_{\beta'}}} \sum_{\substack{(l,m)\,\in\,\beta \\ (l',m')\,\in\,\beta'}} V_{lm,l'm'}\,.$$

The oscillator strength for the exciton ν is proportional to

$$f_\nu = \left[\frac{1}{a}\int_{\Omega_0} \psi^\nu(x,y)\,dxdy\right]^2 = \left[C_{0,0}^{(\nu)}\right]^2 = \left[c_{0,0}^{(\nu)}\right]^2\,. \tag{9}$$

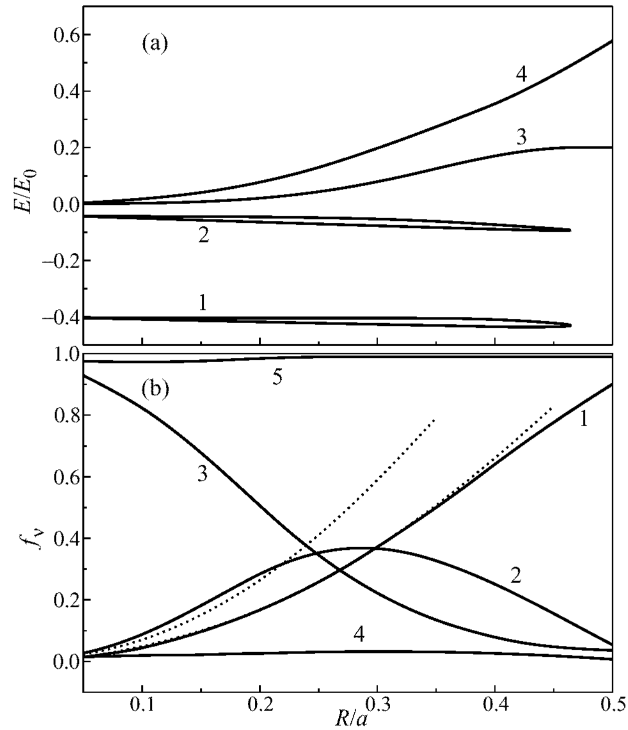

Fig. 1. The energy E_ν (a) and the oscillator strength f_ν (b) of the exciton in a 2D superlattice as a function of the ratio R/a. The calculation is performed for $u_0 = v_0/E_0 = 0.5$; a value of R is being kept fixed while the lateral period a is a variable. The index ν enumerates the exciton Bloch states with $k_x = k_y = 0$; curve 5 in (b) represents the sum of f_ν over the four lowest energy states. Dotted curves are obtained by using the tight-binding approximation, see Eq. (10).

The sum of oscillator strengths is conserved because according to (2) one has $\sum_\nu f_\nu = 1$.

Figures 1 and 2 represent calculations of E_ν and f_ν ($\nu = 1 - 4$) performed for values $u_0 = 0.5$ and $u_0 = 1$. The sum of f_ν over $\nu = 1 - 4$ is represented by curves 5 in Figs. 1b and 2b. Since this sum is close to 1 in the whole range of R/a from 0 up to 0.5, we conclude that the oscillator strengths for excitons with $\nu > 4$ is negligible.

For large enough periods, the exciton states $\nu = 1, 2$ with negative values of E can be approximated by the tight-binding functions

$$\psi^\nu(x, y) = \sum_{lm} \varphi_\nu(x - la, y - ma)\,,$$

where $\varphi_\nu(x, y)$ are the normalized excitonic functions localized at a single potential $v(\rho)$ and characterized by the uniaxial symmetry. In the tight-binding approximation the oscillator strength is given by

$$f_\nu = \frac{1}{a^2}\left(\int \varphi_\nu(x, y)dxdy\right)^2 . \tag{10}$$

Dotted curves in Figs. 1b and 2b are calculated by using Eq. (10). Another important result obtained is that for large a, i.e. for small ratios R/a, the oscillator strength for the exciton $\nu = 3$ is prevailing or, in other words, the state $\nu = 3$ is close to the free exciton state in

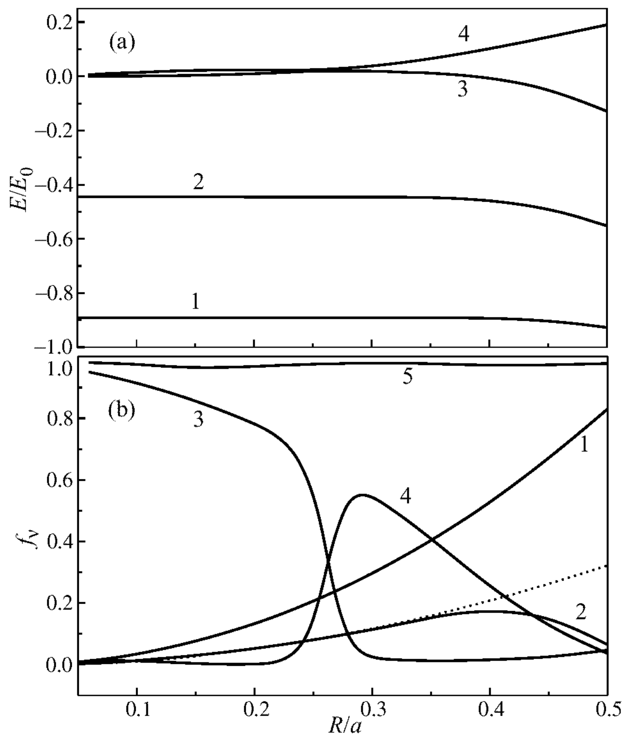

Fig. 2. The same as Fig. 1 but for $u_0 = 1$.

an ideal QW which is described by Eq. (1) with $c_{0,0} = 1$, $c_{lm} = 0$ if $l \neq 0, m \neq 0$ and, therefore, $f = 1$. With increasing R/a the oscillator strength is redistributed in favour of the bound-like states $\nu = 1$ and $\nu = 2$. This redistribution can be used for a qualitative analysis of "stealing oscillator strength" from neutral excitons X to charged excitons X^- mentioned by Kheng et al. [3] (as far as we ignore that the electrons filling the conduction band are not distributed periodically in the interface plane).

The states 3 and 4 in Fig. 2 clearly demonstrate the effect of anticrossing near the point $R/a = 0.25$. In this region the oscillator strengths f_3 and f_4 are linear functions of R/a with the sum $f_3 + f_4$ being constant, at the point $R/a \approx 0.26$ they become equal and the energy difference $E_4 - E_3$ exhibits a minimum, all these properties being fingerprints of the anticrossing effect.

Acknowledgements

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